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The Exploration of the Physical Properties of the Combinations of Selenium-Based Ternary Chalcogenides $AScSe_2$ (A=K, Cs) for Photovoltaic Applications

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Abstract : It is an essential need in this era of Science and Technology to investigate some unique and appropriate materials for optoelectronic applications. Here, we deliberated, for the first time, the structural, optoelectronic, mechanical, vibrational, and thermo dynamical properties of hexagonal structure selenium-based ternary chalcogenides $AScSe_2$ (A= K, Cs) by using Perdew-Burke-Ernzerhof Generalized-Gradient-Approximation (PBE-GGA). The lattice angles for these materials are found as α=β=90o and γ=120o. $KScSe_2$ optimized with lattice parameters a=b=4.3 (Å), c=7.81 (Å) whereas $CsScSe_2$ got relaxed at a=b=4.43 (Å) and c=8.51 (Å). However, HSE06 functional has overestimated the lattice parameters to the extent that for $KScSe_2$ a=b=4.92 (Å), c=7.10 (Å), and $CsScSe_2$ a=b=5.15 (Å), c=7.09 (Å). The energy band gap of these materials calculated via PBE-GGA and HSE06 functionals confirms their semiconducting nature. Concerning Born's criteria, these materials are mechanically stable ones. Moreover, the temperature dependence of thermodynamic potentials and specific heat at constant volume are also determined while using the harmonic approximation. The negative values of free energy ensure their thermodynamic stability. The vibrational modes are calculated by plotting the phonon dispersion and the vibrational density of states (VDOS), where infrared (IR) and Raman spectroscopy are used to characterize the vibrational modes. The various optical parameters are examined at a smearing value of 0.5eV. These parameters unveil that these materials are good absorbers of incident light in ultra-violet (UV) regions and may be utilized in photovoltaic applications.

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